The dynamics of the spherical p-spin model: from microscopic to asymptotic

Bongsoo Kim *, Arnulf Latz †

Institut für Physik, Johannes Gutenberg Universität Mainz, Staudinger Weg 7, D-55099 Mainz, Germany

Abstract

We have numerically investigated the mean-field dynamics of the the p-spin interaction spin glass model with p=3 using an efficient method of integrating the dynamic equations. We find a new time scale associated with the onset of the breakdown of the fluctuation-dissipation theorem in the intermediate time regime. We also find that the off-equilibrium relaxation exhibits a sub-aging behavior in the intermediate times and crosses over to a simple aging in the asymptotic regime.

75.10.Nr, 61.20.Lc, 64.70.pf

*permanent address: Dept. of Physics, Changwon National University, Changwon, 641-773, Korea.

†corresponding author

Since the recognition [1] of possible deep connection between structural glass and some class of spin glass systems such as the p-spin model [2,3], the spherical p-spin model [4], due to its analytic accessibility, has been the subject of intense research in both statics and dynamics. Here we examine some open questions (such as scaling behavior) [5] of the off-equilibrium dynamics of the mean field spherical p-spin model by developing a new method of integrating the dynamic equations of the model.

We consider the system of N spins $S_1, S_2, \cdots S_N$ which interact via Hamiltonian

$$H = -\sum_{1\le i_1<i_2\cdots<i_p\le N} J_{i_1 i_2\cdots i_p} S_{i_1} S_{i_2}\cdots S_{i_p} \tag{1}$$

where the spins are continuous variables subject to the spherical constraint $\sum_{i=1}^{N} S_i^2 = N$. The coupling $J_{i_1 i_2\cdots i_p}$ is a Gaussian random variable with zero mean and variance $[J^2_{i_1 i_2\cdots i_p}]_J = p!/2N^{p-1}$. It is well known [4] that this model (with $p > 2$) exhibits an equilibrium phase transition at a finite temperature $T = T_S$ from paramagnetic phase to spin glass phase characterized by one-step replica-symmetry breaking. This temperature is lower than the than the dynamical freezing temperature T_D, below which the dynamics is non ergodic.

For the time evolution of the system, we consider the following dissipative Langevin dynamics

$$\Gamma^{-1}\partial_t S_i(t) = -z(t)S_i(t) - \frac{\partial H}{\partial S_i(t)} + \eta_i(t) \tag{2}$$

where $z(t)$ is a Lagrange multiplier to enforce the spherical constraint for all times. In order to satisfy the detailed balance, the thermal noise $\eta_i(t)$ is chosen to be Gaussian with zero mean and variance $\langle \eta_i(t)\eta_j(t')\rangle = 2\Gamma^{-1}T\delta_{ij}\delta(t-t')$. The inverse of the kinetic coefficient Γ sets the microscopic time scale, which henceforth is set to unity.

This Langevin dynamics governs the time evolution of the system starting from, for example, the random disordered spin configuration toward thermal equilibrium. Two physical quantities of interest, which quantitatively characterize this time evolution, are the two-time correlation function $C(t,t_w) = \sum_{i=1}^{N}[< S_i(t)S_i(t_w) >]_J/N$ where $\langle\cdots\rangle$ and $[\cdots]_J$ represent averages over thermal noise and random coupling, respectively, and the response function $R(t,t_w) = \sum_{i=1}^{N}[\frac{\partial < S_i(t) >}{\partial h_i(t_w)}]_J/N$ where $h_i(t_w)$ is the external field turned on at time t_w. In equilibrium, these quantities become time-translation invariant, i.e., $C(t,t_w) = C(\tau)$ and $R(t,t_w) = R(\tau)$, $\tau \equiv t - t_w$. Moreover, there exists a fundamental relationship between the correlation and the response, known as the fluctuation-dissipation theorem (FDT), which takes the form for the present irreversible dynamics [6]

$$R(\tau) = -\frac{\theta(\tau)}{T}\frac{\partial C(\tau)}{\partial\tau} \tag{3}$$

where $\theta(\tau)$ is the unit step function which reflects the causality for the response function. We will see below that the non-equilibrium dynamics of the present system manifests an explicit strong dependence of the two times t and t_w (aging) and an interesting modification of FDT [7,4,8].

At this stage, we find it very useful to introduce an integrated response function $F(t,t_w)$ defined as

$$F(t,t_w) \equiv -\int_{t_w}^{t} ds\, R(t,s). \tag{4}$$

From (4) $F(t,t^-)=0$ and $\partial F(t,t_w)/\partial t_w = R(t,t_w)$. FDT (3) then takes the form $F(\tau) = \theta(\tau)[C(\tau)-1]/T$.

In the limit of N going to infinity, one can treat the dynamics exactly using the standard functional method such as Martin-Siggia-Rose formalism [10,1]. In particular, the dynamics is governed by the closed set of coupled equations of C and F:

$$\partial_t C(t,t_w) = -z(t)C(t,t_w) + \frac{p(p-1)}{2}\int_0^t dsC^{p-2}(t,s)(\partial_s F(t,s))C(t_w,s) + \frac{p}{2}\int_0^{t_w} dsC^{p-1}(t,s)\partial_s F(t_w,s), \tag{5}$$

$$\partial_t F(t,t_w) = -1 - z(t)F(t,t_w) + \frac{p(p-1)}{2}\int_{t_w}^t dsC^{p-2}(t,s)(\partial_s F(t,s))F(s,t_w). \tag{6}$$

where $z(t) \equiv T - pE(t)$, $E(t)$ being the average energy per spin. The energy density $E(t)$ is related to C and F as $E(t) = -(p/2)\int_0^t ds\, C^{p-1}(t,s)\partial_s F(t,s)$. The same type of the equations have been derived in various physical contexts such as the dynamics of a long-range superconducting wire network ($p=4$) [11], the dynamics of Amit-Roginsky model($p=3$) [12], and the dynamics of a particle in the random potential in large dimensional space [13–16].

As Cugliandolo and Kurchan (CK) [8] have shown, the dynamics exhibits the two distinct regimes depending on the relative magnitude of the two times $\tau(t \equiv \tau + t_w)$ and t_w. The first regime (while $t, t_w \to \infty$, the time difference $\tau \equiv t - t_w$ is finite, i.e., $\tau/t_w \to 0$) is the regime where the time-translation invariance and FDT hold. That is, $C(\tau+t_w,t_w) = C(\tau)$, $F(\tau+t_w,t_w) = F(\tau)$ and $TF(\tau) = (C(\tau)-1)$ independent of a given t_w. In this regime, the dynamic equation for $C(\tau)$ can be easily derived from the equation for the integrated response and is given by

$$(\partial_\tau + T)C(\tau) + p\left(E_\infty + \frac{1}{2T}\right)(1-C(\tau)) + \frac{p}{2T}\int_0^\tau dsC^{p-1}(\tau-s)\frac{dC(s)}{ds} = 0. \tag{7}$$

where E_∞ is the long time limit of the energy density $E(t)$, $E_\infty \equiv \lim_{t\to\infty} E(t)$. One can recognize that this equation is quite similar to a schematic model developed in the context of the mode-coupling theory (MCT) for the glass transition in structural glasses [17]. In particular, apart from the term involving $(1-C(\tau))$, (7) with $p=3$ is identical to the Leutheusser model (without the inertial term) [18]. Hence one can sense that this equation, as in the Leutheusser model, may lead to a dynamic transition to a nonergodic phase where the long-time limit of $C(\tau)$ is non-vanishing. It is easy to show from (7) that the non-ergodicity parameter $q \equiv \lim_{\tau\to\infty} C(\tau)$ is then related to E_∞ via

$$-(T - pE_\infty) + \frac{p}{2T}(1-q^{p-1}) = -\frac{T}{1-q} \tag{8}$$

But the full understanding of the FDT dynamics requires the asymptotic value of the energy density, E_∞, for which one has to consider the dynamics in different regime (aging regime); the two regimes are closely coupled to each other.

When the two times t and t_w are large and well separated, the relaxation is very slow, and hence the time derivatives in (5) and (6) can be ignored. In this situation, it is found that the scaling Ansatz for C and F

$$C(t, t_w) = \mathcal{C}\left[\frac{h(t_w)}{h(t)}\right], \quad F(t, t_w) = \mathcal{F}\left[\frac{h(t_w)}{h(t)}\right] \tag{9}$$

leads to

$$\frac{p(p-1)}{2T^2}(1-q)^2 q^{p-2} = 1, \tag{10}$$

$$T\mathcal{F}(\lambda) = x\mathcal{C}(\lambda) - [1 - (1-x)q], \tag{11}$$

and

$$E_\infty = -\frac{1}{2T}\left[1 - (1-x)q^p\right] \tag{12}$$

with $x = (p-2)(1-q)/q$ for non vanishing q. The equation (11) with $x < 1$ is a modification of FDT in aging regime and is one of the most important results obtained from the asymptotic analysis. Note that although the actual dynamics will select the form of $h(t)$ uniquely, the above asymptotic analysis holds for an arbitrary monotonically increasing function $h(t)$ (known as the time-reparametrization invariance): the function $h(t)$ remains undetermined within the asymptotic analysis.

We now go back to the equation (7) and discuss the dynamics of FDT regime. First note from (8) that $q = 0$ is always a solution for all temperatures. We see from (10) that the non-vanishing q starts to appear at the temperature $T^* = [2p^{1-p}(p-1)(p-2)^{p-2}]^{1/2}$ at which $q = q^* = (p-2)/p$ ($q^* = 1/3$ and $T^* = 2/3$ for $p = 3$). Thus below T^*, starting from the initial state with *zero* energy density [19] (*e.g.*, the state with all spins up), the system always chooses the solution with *higher* energy (which is the highest TAP state at a given T [8,20–22]) among these two solutions. Thus for $T_D < T \le T^*$, $q = 0$ is the genuine solution, and $E_\infty = -1/(2T)$, $x = 1$. The system is ergodic. The dynamic transition temperature T_D is determined by $x(T = T_D) = 1$ for $q \ne 0$. This condition with (10) lead to $q_D = (p-2)/(p-1)$ and $T_D = [p(p-2)^{p-2}/(2(p-1)^{p-1})]^{1/2}$ (for $p = 3$, $T_D = \sqrt{3/8} \simeq 0.612\cdots$ and $q_D = 1/2$). Therefore the term involving $(1 - C(\tau))$ drops out in (7) and the resulting equation is the same as a schematic mode-coupling equation for supercooled liquids. Therefore the relaxation dynamics above the dynamic transition exhibits the well-known scaling laws derived with MCT [23]. For $T \le T_D$ the system chooses $q \ne 0$, $x < 1$, and $E_\infty + 1/(2T) > 0$. Hence the system is non-ergodic. Thus the term $p(E_\infty + 1/2T)(1 - C(\tau))$ in (7) is turned on. This additional term makes the dynamics in the FDT regime in the present model differ from that of the MCT for supercooled liquids. In particular, near the transition $q(T)$ shows a linear behavior $q(T) = q_D + \text{const.}(T_D - T)$ instead of a square-root singularity observed in MCT. Also whereas the critical relaxation is seen very near and at the transition in MCT, in the present situation the correlation exhibits a critical relaxation $C(\tau) = q + \text{const.}\tau^{-a}$ for *all* temperatures below the transition with the exponent a related to the FDT violating factor x as $\Gamma^2[1-a]/\Gamma[1-2a] = x/2$ [15], Γ being the gamma function.

Though the asymptotic analysis put forward by CK provided quantitative informations on the both FDT and the asymptotic aging dynamics, it leaves unexplored the non-equilibrium dynamics in the intermediate time regime. Moreover, the time reparametrization invariance leaves undetermined the form of the function $h(t)$ which the original set of causal dynamic equations would select in the course of its evolution. Therefore, we do not know what type of scaling feature the long time aging dynamics might exhibit.

In this work, we have developed an efficient way of integrating the mean-field dynamic equations (5) and (6), which can extend the solution to the time regime long enough so that one can clearly investigate the aforementioned important open questions. Basic idea is that since the relaxation becomes very slow at long times one can employ an adaptive integration time step [24]. There are two crucial ingredients in the present method. First, one has to work with the integrated response instead of the response function since the integrated response relax much more slowly than the response (which is basically a time derivative of the correlation). Another ingredient is to increase the integration time step along the both two time directions in such a way that the fast relaxing time regime should have many integration points. The details of the present method will be given elsewhere.

Now we turn to the discussion of the numerical results. All presented results are for $p = 3$. Here we focus on the dynamics below the transition. Shown in Fig. 1(a) is C and F for $T = 0.5$. Both functions exhibit a strong t-dependence (aging effect) which persists up to longest time t. In contrast to the situation above the transition, here the aging will not be interrupted, and the system remains perennially out-of-equilibrium. The parametric plot $-TF(t, t-\tau)$ versus $C(t, t-\tau)$ for $T = 0.5$ shown in Fig. 2(b) exhibits several interesting features. After some time $t \sim 10^2$, independent of time t, the FDT is established in the range $q \le C \le 1$. Then, after still longer time $t \sim 10^5$, all the curves with different times t merge into a single straight line with slope close to the FDT violation parameter $x \simeq 0.565\cdots$. Note the huge time interval (more than 9 decades!) it takes to reach the asymptotic regime. Therefore in the asymptotic regime, the FDT and its violation can be characterized by the two straight lines with slopes 1 and x meeting at $C = q$: $-TF = 1 - C$ for $q \le C \le 1$ and $-TF = x(1-C) + (1-x)(1-q)$ for $C \le q$. This is in accordance with the result of the asymptotic analysis (11). Similar breakdown of FDT has been observed in simulations of supercooled liquids [25–27] and spin glass [28].

One interesting new feature we find in the off-equilibrium dynamics in the intermediate time region is the existence of a new time scale associated with the onset of FDT violation. Note that the breakdown of FDT occurs sharply at $C = q$ (see Fig. 2(b)). Hence we are able to measure this time scale by reading off the times τ_p defined as $C(t, t-\tau_p) = q$ for each fixed t. The double-log plot τ_p versus t in the inset of Fig. 2(a) indeed demonstrates that τ_p shows a power law dependence on t as $\tau_p \sim t^{\phi}$ with $\phi \simeq 0.68$. Furthermore, the big difference in τ_p and t for large t implies that $\tau_p \sim t_w^{\phi}$ with the same exponent. Since ϕ is smaller than 1, we find a new time scale characterizing the aging dynamics in intermediate time region. It is thus highly desirable to have a theoretical development which can provide a detailed information on the dynamics in the intermediate times and on the crossover to the asymptotic time regime. The presence of this time scale in the spherical SK model ($p = 2$) was demonstrated by Zippold et al [29].

We now discuss the scaling behavior in the aging regime. Recall that the asymptotic analysis loses information on the unique selection of $h(t)$. The scaling property in our

numerical solution is important since it will be able to determine the specific form of the function $h(t)$ that the system actually selects. Figure 2(a) shows the relaxation of the correlation function $C(\tau + t_w, t_w)$ for different waiting times t_w at $T = 0.5$. Due to the adaptive integration steps along the both t and t_w axes, it is inevitable that the short time data for each fixed t_w is lost. It is natural to first examine the possibility of $h(t)$ being a power of t, $h(t) \sim t^{\gamma}$. This means that the correlation in the aging regime shows a scaling behavior $C_A(\tau + t_w, t_w) = \hat{C}(\tau/t_w)$ (known as the simple aging). To check this scenario, we plot in Fig. 2(b) the correlation function $C(\tau + t_w, t_w)$ against the rescaled time τ/t_w. Indeed, we observe that the relaxation data with longest waiting times collapse onto a single scaling curve. Thus we find that the relaxation obeys the simple aging in the asymptotic time regime. It is also very interesting to observe that the relaxation in the intermediate waiting times exhibit a sub-aging behavior (the characteristic relaxation time grows slower than the waiting time), which is often observed [30]in the experimental data of thermoremanent magnetization (TRM) of real spin glass systems. Note that the crossover from the sub-aging to the simple aging occurs over a rather broad time region. We find that close to the dynamic transition, as shown in Fig. 3(a), the simple scaling is not yet fulfilled for waiting times which are long enough to reach simple aging at $T = 0.5$. This suggests that the crossover time from sub-aging to simple aging becomes broader as the transition is approached.

Though the sub-aging eventually makes a crossover to the simple aging behavior, due to the broadness of the crossover regime (particularly near the transition), we wanted to know whether there is a scaling function $h(t)$, which can collapse the data in the intermediate times. One available empirical form is $h(t) = \exp[\frac{1}{1-\mu}(t/t_0)^{1-\mu}]$, which has been successfully used to collapse the TRM data in spin glasses [30]. The time t_0 is the microscopic time scale ($t_0 = 1$ for our case). The case of $\mu = 0$ corresponds to the absence of aging (no waiting time dependence), and the case of $\mu = 1$ to the simple aging. Thus, the sub-aging behavior will give $0 < \mu < 1$. As shown in Fig. 3(b), with this empirical form of $h(t)$ with $\mu \simeq 0.81$ for $T = 0.61$, we can collapse *both* the correlation and the integrated response with largest waiting times. We find that the exponent μ becomes larger in order to collapse the sub-aging data (with the same range of waiting times) at lower temperatures. We should emphasize that μ is an *effective* exponent, i.e., it tends to *increase* in order to incorporate the data with longer waiting times into scaling collapse due to the crossover to simple aging.

In summary, we have developed an efficient method of integrating the dynamic equations of a mean field spin glass model with p-spin interaction. This method allows us to see numerically for the first time the entire dynamic regime covering from microscopic to asymptotic regime. Tio cover such a broad dynamic range will also be of major importance in the sudy of aging in structural glasses [31]. We observe several new dynamic features in the intermediate time regime including the existence of a new time scale at which the breakdown of FDT sets in, the broad sub-aging regime and its crossover dynamics to the simple aging. These findings offer a new theoretical challenge for further understanding of the off-equilibrium dynamics of the p-spin model.

ACKNOWLEDGMENTS

We thank K. Binder, L. Cugliandolo, H. Horner, K. Kawasaki, W. Kob, J. Kurchan, M. Mézard, R. Schilling and T. Theenhaus for valuable discussions and suggestions. B.K. thanks R. Schilling and K. Binder for hospitality during his sabbatical at Mainz. This work was supported by the SFB 262 and the MWFZ of the Johannes Gutenberg-University of Mainz.

REFERENCES

[1] Kirkpatrick T. R. and Thirumalai D., Phys. Rev. B **36** (1987) 5388.
[2] Derrida B., Phys. Rev. Lett. **45** (1980) 79; Phys. Rev. B. **24** (1981) 2613.
[3] Gross D. J. and Mézard M., Nucl. Phys. B **240** (1984) 431.
[4] Crisanti A. and Sommers H. J., Z. Phys. B **87** (1992) 341; Crisanti A., Horner H. and Sommers H. J., Z. Phys. B **92** (1993) 257.
[5] Bouchaud J. -P., Cugliandolo L. F., Kurchan J. and Mézard M., Spin Glasses and Random Fields, A. P. Young, World Scientific, Singapore (1998).
[6] Deker U. and Haake F., Phys. Rev. A **11** (1975) 2043.
[7] Horner H., Z. Phys. B **87** (1992) 291.
[8] Cugliandolo L. F. and Kurchan J., Phys. Rev. Lett. **71** (1993) 173; J. Phys. A 27 (1994) 5749; Phil Mag. B **71** (1995) 50.
[9] Bouchaud J. -P., Cugliandolo L. F., Kurchan J. and Mézard M., Physica A **226** (1996) 243.
[10] Martin P. C., Siggia E. D. and Rose H. A., Phys. Rev. A **8** (1973) 423.
[11] Chandra P., Feigelman M. V., Ioffe L. B., and Kagan D. M., Phys. Rev. B **56** (1997) 11553.
[12] Franz S. and Hertz J., Phys. Rev. Lett. **74** (1995) 2114.
[13] Kinzelbach H. and Horner H., J. Phys.I (France) **3** (1993) 1392; J. Phys.I (France) **3** (1993) 1901.
[14] Franz S. and Mézard M., Europhys. Lett. **26** (1994) 209; Physica A **210** (1994) 48.
[15] Cugliandolo L. F. and Le Doussal P., Phys. Rev. E **53** (1996) 1525.
[16] Horner H., Z. Phys. B **100** (1996) 243.
[17] Bengtzelius U., Götze W. and Sjölander A., J. Phys. C **17** (1984) 5915; Götze W., Liquids, freezing and glass transition, Hansen J. P., Levesque D. and Zinn-Justin J., Les Houches (1989.
[18] Leutheusser E., Phys. Rev. A **29** (1984) 2765.
[19] For the different situations, see Barrat A., Burioni R. and Mézard M., J. Phys. A **29** (1996) L81.
[20] Kurchan J., Parisi G. and Virasoro M. A., J. Phys. I **3** (1993) 1819.
[21] Crisanti A. and Sommers H. J., J. Phys. I **5** (1995) 805.
[22] Franz S. and Parisi G., J. Phys. I **5** (1995) 1401.
[23] Götze W., Z. Phys. B **60** (1985) 195.
[24] Fuchs M., Götze, Hofacker H. and Latz. A, J. Phys. Condensed Matter **3** (1991) 5047.
[25] Parisi G., Phys. Rev. Lett. **79** (1997) 3660.
[26] Kob W. and Barrat J. -L. , Phys. Rev. Lett. **78** (1997) 4581; Barrat J. -L. and Kob W., Europhys. Lett. **46** (1999) 637; Kob W. and Barrat J. -L. Preprint cond-mat/9905248.
[27] Di Leonardo R., Angelani L., Parisi G. and Ruocco G, Preprint cond-mat/0001311.
[28] Rieger H. and Franz S., J. Stat. Phys. **79** (1995) 749; Marinari E., Parisi G., Ricci-Tersenghi F. and Ruiz-Lorenzo J. J., J. Phys. A **31** (1998) 2611.
[29] Zippold W., Kühn R. and Horner H., Preprint cond-mat/9904329.
[30] Vincent E., Hammann J., Ocio M. and Bouchaud J. -P., Proceedings of the Sitges Conference on Glassy Systems, E. Rubi, Springer, Berlin (1996).
[31] Latz A., J. Phys. Condens. Matt. (in print); preprint, cond-mat/9911025.

FIGURES

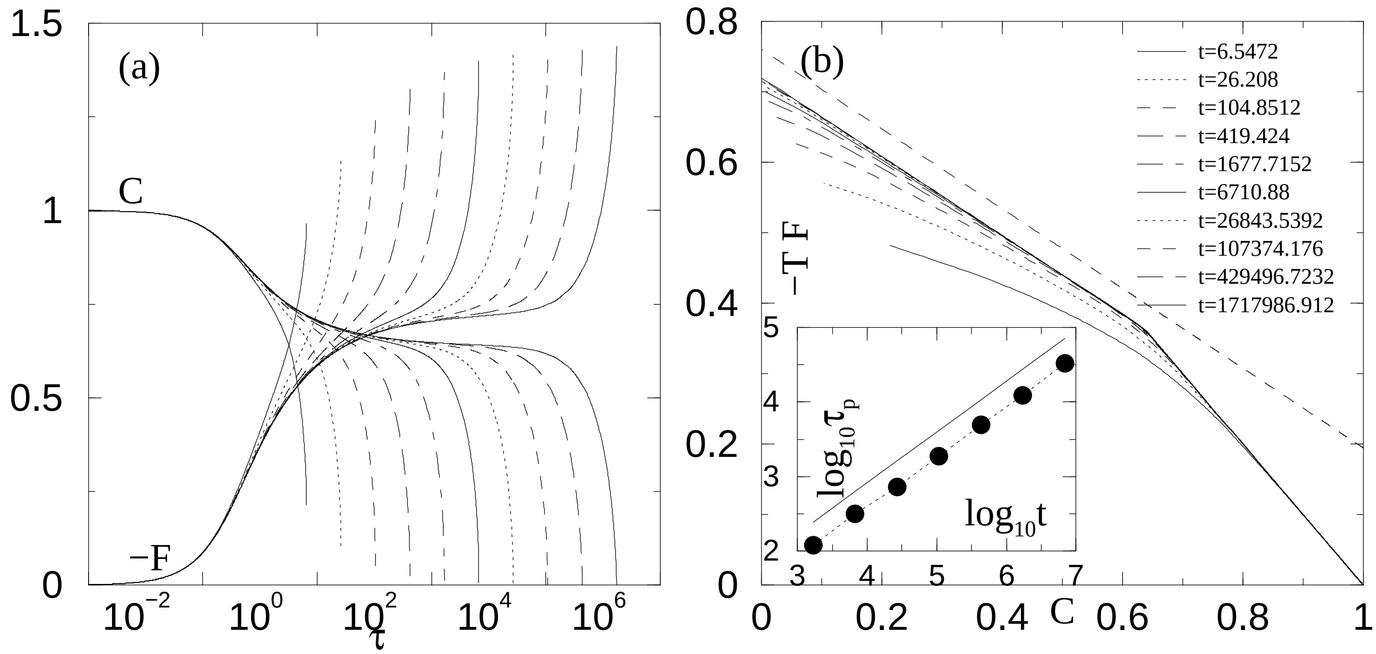

FIG. 1. (a) The correlation function $C(t, t-\tau)$ and the integrated response function $F(t, t-\tau)$ versus τ with different t for $T = 0.5$. (b)The parametric plot $-TF(t, t-\tau)$ versus $C(t, t-\tau)$ with different t as in (a). The dashed straight line with slope -0.565 is shown for comparison. Inset: τ_p versus t in a log-log plot. The solid straight line with slope 0.68 is shown for comparison.

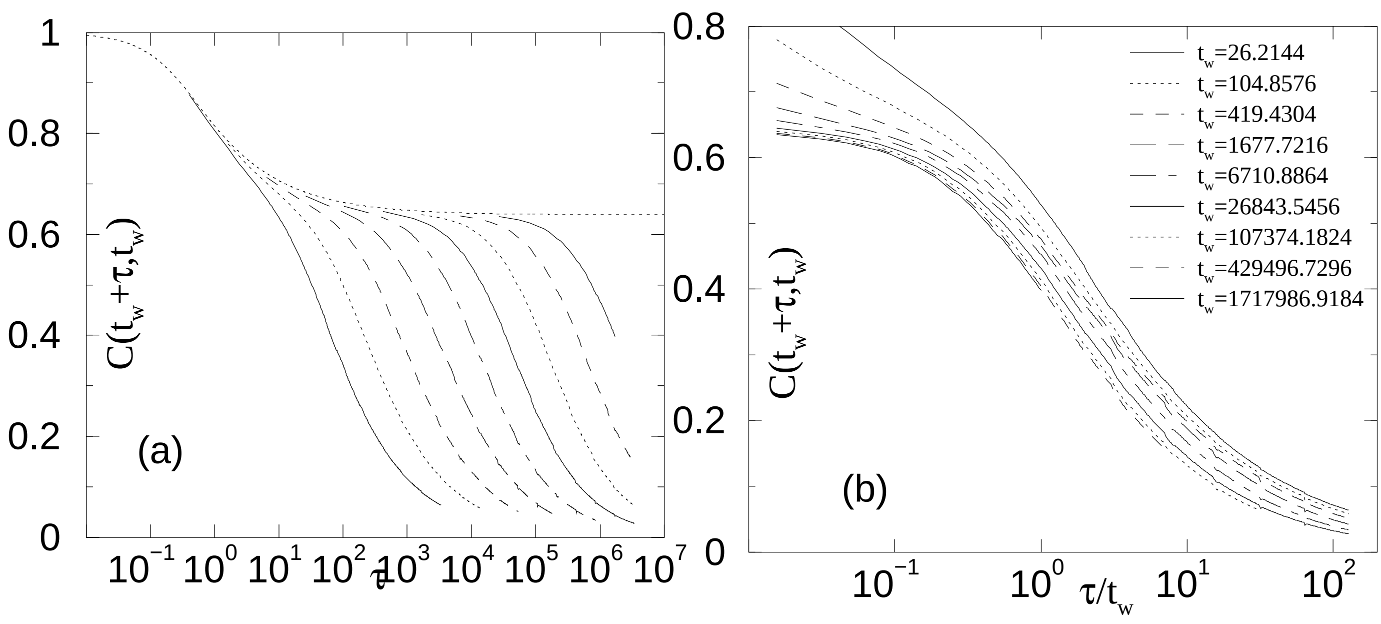

FIG. 2. (a) The correlation function $C(t_w + \tau, t_w)$ versus τ for different waiting times t_w at $T = 0.5$. The upper dotted line is the numerical solution of (7). (b) $C(t_w + \tau, t_w)$ versus rescaled time τ/t_w for the data shown in (a).

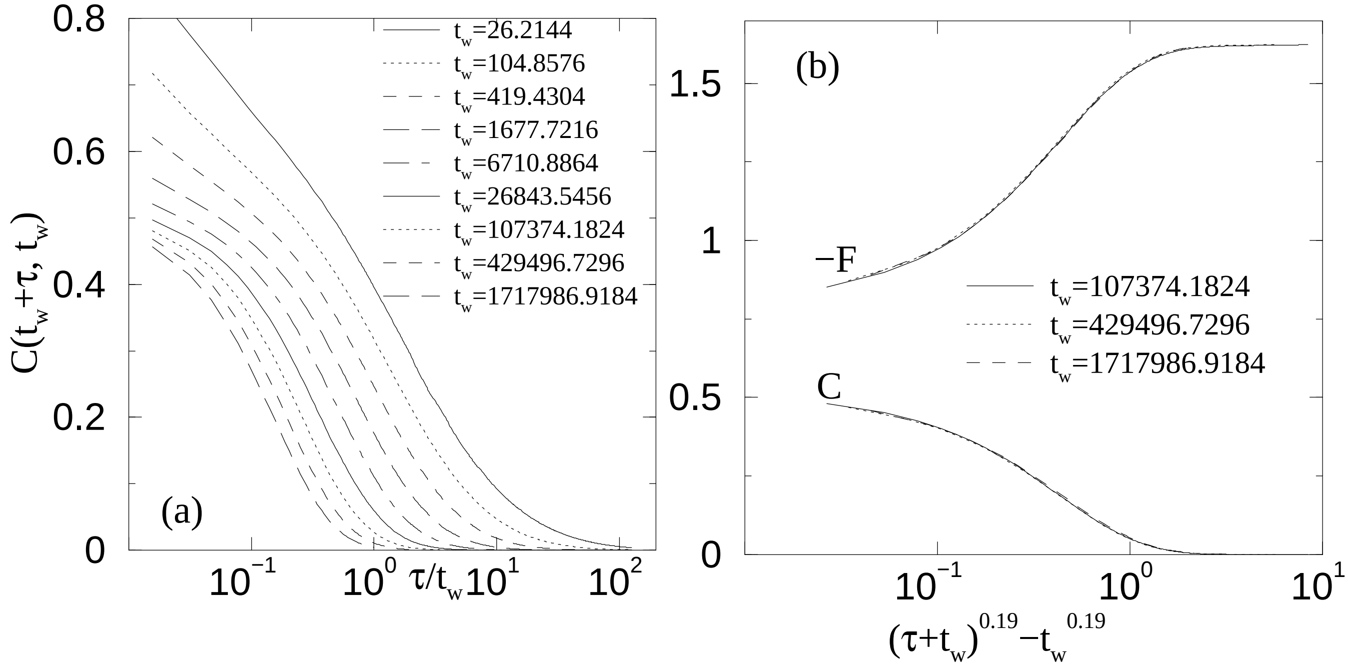

FIG. 3. (a)$C(t_w+\tau, t_w)$ versus rescaled time τ/t_w for $T = 0.61$. (b) Scaling plot for $C(t_w+\tau, t_w)$ and $F(t_w + \tau, t_w)$ for $T = 0.61$ using $h(t) = \exp[t^{1-\mu}/(1-\mu)]$ with $\mu = 0.81$.